2,3,4-Trinitrotoluene
602-29-9 | DTXSID60208944

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.94e-03 mol/L

Global applicability domain: Outside

Local applicability domain index: 3.09e-01

Confidence level: 4.65e-01

Nearest Neighbors from the Training Set

Image not found
Methane, bromotrinitro-
Measured: 1.70e-02
Predicted: 1.38e-02

Image not found
2,4,6-Trinitrotoluene
Measured: 5.72e-04
Predicted: 3.38e-03

Image not found
1,2-Dinitrobenzene
Measured: 7.91e-04
Predicted: 2.41e-03

Image not found
Pentaerythritol tetranitrate
Measured: 1.36e-04
Predicted: 2.73e-04